

# Simulations of Heat and Oxygen Transport in a Nuclear Fuel Element

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Uranium oxide ( $\text{UO}_{2+x}$ )-based nuclear fuels are commonly used in thermal, light-water reactors and have been recently considered as the potential fuel for fast breeder reactors. The oxide nuclear fuel rods consist of oxide fuel pellets stacked in a cylindrical metal cladding and then bundled in a fuel assembly (Fig. 1) [1] operating at temperatures of up to 2000 K. In this work we examine the influence of temperature and stoichiometry changes on the  $\text{UO}_{2+x}$  fuel properties and on the coupling of heat and species transport in a fuel element with stainless steel cladding. The objective is to improve the understanding of fuel damage and performance.

In a nuclear reactor, irradiation induces changes in material properties such as microstructure, density, thermal conductivity, specific heat, and oxygen diffusivity. We have developed models of these properties that provide correlations with temperature, pressure, burnup, and other reactor parameters [2,3]. As opposed to common approaches, our models include the dependence of the properties on the stoichiometry  $x$  in  $\text{UO}_{2+x}$ .

The finite element simulations of coupled heat and oxygen transport were performed using COMSOL Multiphysics®, which provides an ideal tool for studying coupled phenomena and allows for mesh and time step refinement in 3D configurations (Fig. 2). To solve the heat and species equation, we employed quadratic Lagrange elements and a nonlinear iterative technique with a nested unsymmetric multifrontal (UMFPACK) linear solver.

Our steady-state parametric studies were focused on determining the centerline temperature in the fuel rod as a function of non-stoichiometry and the rate of heat generation during fission. Given the strong temperature gradients in the reactor, we have included the effect of the thermally driven diffusion of species, also known as the Soret effect. We proved that the counterbalancing of the Soret and Fickian fluxes is responsible for the variation of oxygen concentration in the fuel pellet [4]. The simulations show that including the dependence of thermal conductivity

and density on non-stoichiometry can lead to changes in the calculated centerline temperature and thermal expansion displacements that exceed 5% (Fig. 3).

We have also simulated transient regimes and examined the time lag in the response of the temperature and non-stoichiometry distributions with respect to sudden changes in heat generation rate intensity and oxygen removal rate. Future work will include studies on the effects of porosity and simulations of fuel-cladding interactions.

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- [1] United States Nuclear Regulatory Commission, Emergency Preparedness web page: <http://www.nrc.gov/about-nrc/emerg-preparedness/images/fuel-pellet-assembly.jpg>
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- [3] M. Stan, et al., *J. Alloys Comp.*, **444-445**, 415-423 (2007).
- [4] J. C. Ramirez, M. Stan, and P. Cristea, *J. Nucl. Mater.*, **359**, 174-184 (2006).

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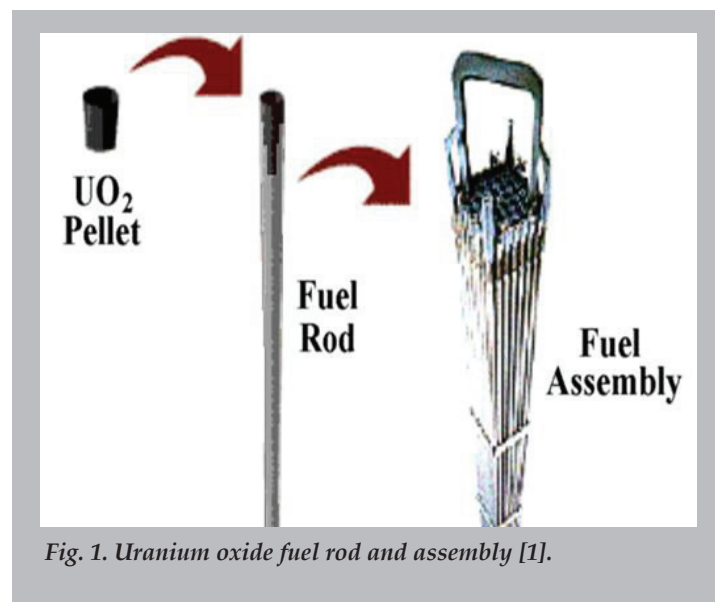


Fig. 1. Uranium oxide fuel rod and assembly [1].

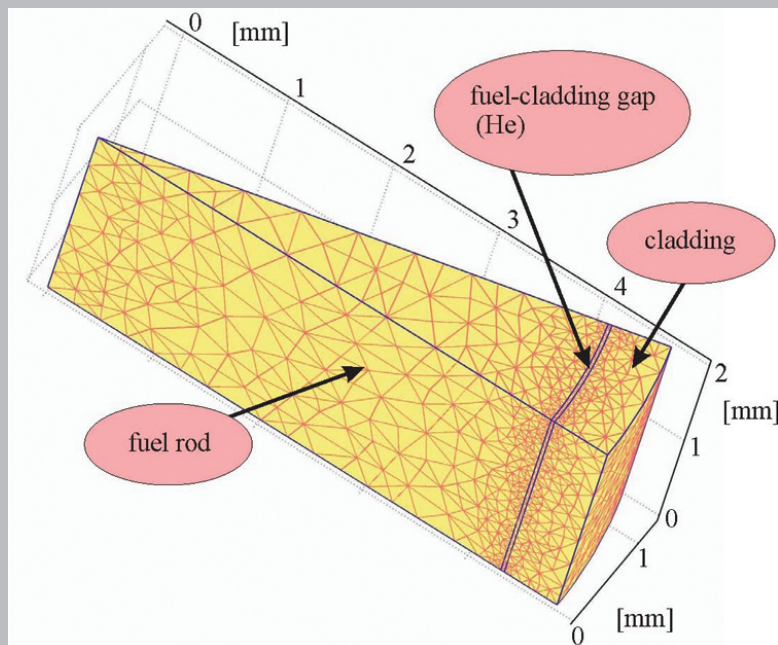


Fig. 2. Representative "slice" of the computational domain, showing a 22.5 deg. angular sector of the fuel element. The mesh was refined at the gap, where temperature and stoichiometry gradients are steeper.

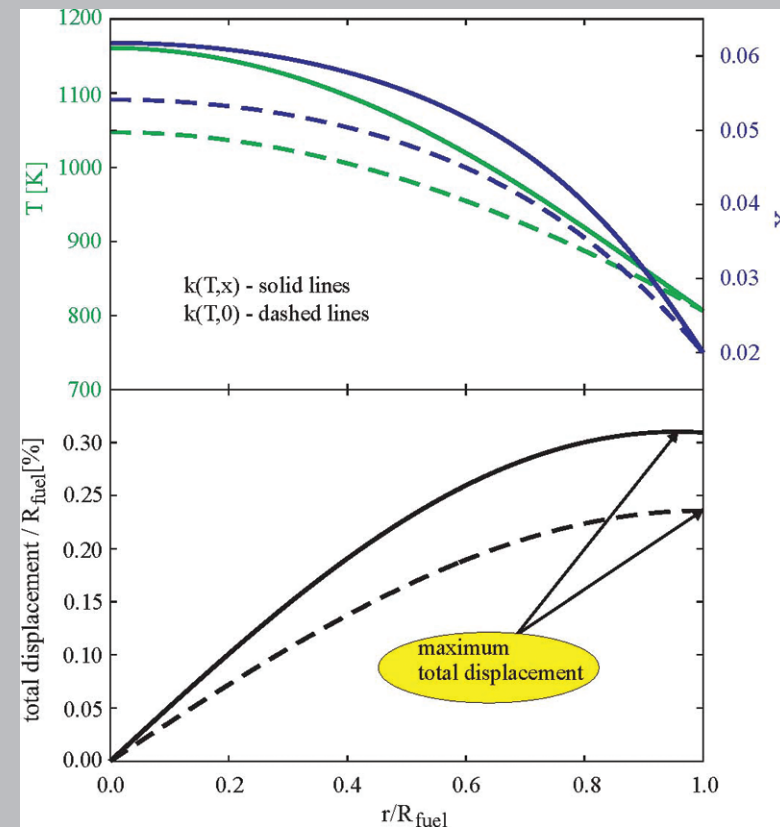


Fig. 3. Top: Steady-state temperature (blue) and non-stoichiometry (green) distribution in radial direction for a  $\text{UO}_{2+x}$  fuel rod. Note the significant changes introduced by including the stoichiometry dependence of the thermal conductivity in the simulation (solid lines) compared to temperature dependence only (dashed lines). Bottom: Thermally induced expansion (displacement) of the fuel element. Note the changes introduced by including the stoichiometry dependence and the position of the maximum total displacement inside the fuel pellet. This is consistent with experimentally observed angular cracks.